

Supplementary data for the article:

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Table S1. Composition of stock solutions and simulated digestion fluids SSF-simulated salivary fluid, SGF-simulated gastric fluid, SIF- simulated intestinal fluid. All simulated fluids were prepared as 1.25× concentrates since the subsequent addition of enzymes, bile salts, Ca^{2+} solution, and water will result in the correct concentration of each compound in the final digestion mixture.

Compound	Stock conc.		SSF	SGF	SIF
			pH 7.0	pH 3.0	pH 7.0
			Conc. in SSF	Conc. in SGF	Conc. in SSF
	g/L	mol/L	mmol/L	mmol/L	mmol/L
KCl	37.3	0.5	15.1	6.9	6.8
KH_2PO_4	68	0.5	3.7	0.9	0.8
NaHCO_3	84	1	13.6	25	85
NaCl	117	2	-	47.2	38.4
$\text{MgCl}_2(\text{H}_2\text{O})_6$	30.5	0.15	0.15	0.1	0.33
$(\text{NH}_4)_2\text{CO}_3$	48	0.5	0.06	0.5	-
NaOH	-	1	-	-	8.4
HCl	-	6	1.1	15.6	-
* $\text{CaCl}_2 (\text{H}_2\text{O})_2$	44.1	0.3	0.75*	0.075*	0.3*

* Concentrations refer to the final digestion mixture, $\text{CaCl}_2 (\text{H}_2\text{O})_2$ was added separately.

Table S2.

Molecular ions of the tested polyphenols together with the two most intense fragments from the MS² spectra and the specific collision energy at which they are formed.

Phenolic compounds	Parent Ion, <i>m/z</i>	Product Ion, <i>m/z</i> (Collision Energy, <i>eV</i>)
<i>Phenolic acid</i>		
5- <i>O</i> -caffeoylquinic acid	353.103	191.28 (25)
<i>p</i> -hydroxybenzoic acid	137.057	93.19 (19); 108.33 (22)
<i>p</i> -coumaric acid	163.031	93.12 (39); 119.09 (16)
Vanillic acid	167.034	108.00 (21); 153.00 (15)
Ferulic acid	193.057	134.00 (18); 178.00 (15)
<i>Flavonols</i>		
Quercetin-3- <i>O</i> -glucoside	463.002	271.01 (44); 300.02 (29)
Quercetin-3- <i>O</i> -rhamnoside	447.011	300.08 (38); 301.10 (28)
Rutin	609.197	299.98 (42); 301.20 (32)
Isohramnetin-3- <i>O</i> -glucoside	477.009	314.02 (28); 314.98 (36)
Kaempferol-7- <i>O</i> -glucoside	447.088	257.03 (40); 285.03 (30)
<i>Other phenolics</i>		
Apigenin	269.032	117.24 (43); 149.00 (24)
Naringenin	271.036	119.10 (25); 151.07 (19)
Naringin	579.241	151.42 (43); 217.26 (33)
Eryodictiol	287.069	107.08 (15); 151.25 (25)